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A Modification Technique of Collision Probability in the Direct Simulation Monte Carlo Method

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Abstract

In Direct Simulation Monte Carlo (DSMC) method, it is difficulty to keep grid size smaller than local mean free path, that influences calculation accuracy much. In this paper, a new modification technique of collision probability with least square method and sub-relaxation technique is introduced to improve simulation accuracy in DSMC with coarse grid size. The new method is applied to direct simulation Monte Carlo method based on unstructured tetrahedral cells, which can be easily used for other grid topology. A numerical example with different grid size is implemented to validate the method discussed here, and the numerical results confirm feasibility of the modification technique.

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Keywords: DSMC; Unstructured grid; Collision probability correction; Least square method

1. Introduction

As the development of hypersonic vehicles, star exploration and satellite technique[1-3], rarefaction becomes more and more important. In numerical simulation methods for forecasting the rarefied aerodynamics, Direct Simulation Monte Carlo(DSMC) method is the most effective one than others[4,5]. Direct simulation Monte Carlo(DSMC)method had been formulated by Bird [6] in 1970,and it marked a milestone in the evolution of fluid mechanics. Although probably not appreciated then, the method had enormous power, and, as time went on, it was

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extensively adopted at solving very complex rarefied flows involving chemical reactions, ionization, and high degrees of molecular non-equilibrium [4,5]. The basic steps in DSMC[6] simulation are that the position, velocity, and internal energy of each simulated particle which represent real gas particles are stored and can be changed as colliding with each other and reflecting off surfaces. Lastly, the macroscopic quantities of the flow can be obtained by sampling.

One of the fundamental assumptions of the DSMC method is that particle movement can be decoupled from collision behavior. The probability of a collision occurring is dependent on the collision model and selection scheme being employed and is a function of the relative velocity, collision cross section and the gas number density in that cell.

No time counter (NTC) scheme of Bird[7] for collision pair selection in the Direct Simulation Monte Carlo (DSMC) is used to determine the number of potential collision pairs in a cell. The number of potential collision pairs in a cell is related to the cell-averaged number density, and collision probability for each pairs is not related to local position within a cell. However, when grid size is coarse, internal density variation within a cell will introduce collision probabilities error if using the cell-averaged number density for collision probability. Correction of the binary collision probability for effects of spatial density variation need to be done.

From above all, collision probability of potential collision pairs in a coarse cell is very different from that in a dense grid cell. To correct the collision probabilities error of a collision pairs in a coarse cell, linear reconstruction for number density in a cell can be made, and local collision probability of the collision pairs in a cell can be modified with local number density. Burt[8] has used this method in Cartesian grid. However, it can be found that Burt's method is easy to use in Cartesian grid, but that is difficult for other mesh topology. In this paper, this difficulty can be overcome by using least square method and sub-relaxation method.

2. Present approach

2.1 DSMC methods[6]

The variable hard sphere model was used for molecular collisions. The Larsen-Borgnakke model[9] was assumed for energy transfer between translational and internal molecular modes. The rotational energy was only considered in the internal modes. The acceptance-rejection method was applied for the division of energy. Diffuse reflection condition is used at wall.

2.2 collision probability correction method

For NTC methods, the number of collisions in Δt time step is computed by

$$N_{coll} = \frac{W\bar{N}^2}{2V} \Delta t (\sigma g)_{\max} \quad (1)$$

Where σ is collision cross section, g is relative velocity, \bar{N} is the time-averaged molecular number, N_{coll} is collisions number, Δt is time step, W is particle weight, V is cell volume.

In DSMC method, the collision probabilities of a collision pairs in a cell is given by

$$p_{ij} = \frac{\sigma_{ij} g_{ij}}{(\sigma g)_{\max}} \quad (2)$$

Substituting Eqs. (1-2) to Eq. (3), the averaged collision frequency in a cell can be computed by

$$\begin{aligned}
 F(x) &= \frac{2}{\bar{N}\Delta t} \langle N_{coll} P_{ij} \rangle \\
 &= \frac{W\bar{N}}{V} \langle \sigma_{ij} g_{ij} \rangle = n_c \langle \sigma_{ij} g_{ij} \rangle
 \end{aligned} \quad (3)$$

It can be found from Eq.(3), local number density $n(x) \neq \frac{W\bar{N}}{V}$ in a coarse cell, when using averaged number density $n_c = \frac{W\bar{N}}{V}$ to solve collision frequency, error will be introduced.

While linear number density distribution in a cell is used, number density is given by

$$n(\mathbf{x}) = n_c + \nabla n^Q(\mathbf{x} \square \mathbf{x}_c) \quad (4)$$

Here, \mathbf{x}_c is cell center positions, n_c is number density in cell center.

For correcting Eq.(3), Eq.(2) can be firstly corrected by number density ratio. That is given by

$$p_{ij} = \frac{\sigma_{ij} g_{ij}}{(\sigma g)_{\max}} \frac{n(\mathbf{x})}{n_c}, \text{ Substituting Eq. (4) to this, it can be computed by}$$

$$p_{ij} = \frac{\square_{ij} g_{ij}}{(\square g)_{\max}} (1 + \nabla n^Q(\mathbf{x}_{ij} \square \mathbf{x}_c)) \quad (5)$$

Here $\mathbf{x}_{ij} = (m_i \mathbf{x}_i + m_j \mathbf{x}_j) / (m_i + m_j)$, m_i is molecule mass, \mathbf{x}_i is the coordinates of molecule i. It can be found from Burt's result that ∇n is easy to be solved in Cartesian grid, and it is difficult with other grid methodologies such like structured grid, unstructured grid. In this paper, least square method and sub-relaxation technique are used to overcome the difficulty. For an unstructured tetrahedron cell, there are four neighbor cells (three neighbors for boundary cell). It can be defined by $f = \sum_{i=1}^4 (n(\mathbf{x}) - n_c^i)^2$, here, n_c^i is number density of neighbors.

When extremum of the variable f exist, it can be defined by $\frac{\partial f}{\partial(\frac{\partial n}{\partial x})} = \frac{\partial f}{\partial(\frac{\partial n}{\partial y})} = \frac{\partial f}{\partial(\frac{\partial n}{\partial z})} = 0$

Linear equations about $\frac{\partial n}{\partial x}$, $\frac{\partial n}{\partial y}$, $\frac{\partial n}{\partial z}$ can be written as

$$\frac{\partial n}{\partial x} \sum_{i=1}^4 (x_i - x_c)^2 + \frac{\partial n}{\partial y} \sum_{i=1}^4 [(x_i - x_c)(y_i - y_c)] + \frac{\partial n}{\partial z} \sum_{i=1}^4 [(x_i - x_c)(z_i - z_c)] = \sum_{i=1}^4 [(x_i - x_c)(n_c^i - n_c)]$$

$$\frac{\partial n}{\partial x} \sum_{i=1}^4 [(x_i - x_c)(y_i - y_c)] + \frac{\partial n}{\partial y} \sum_{i=1}^4 (y_i - y_c)^2 + \frac{\partial n}{\partial z} \sum_{i=1}^4 [(y_i - y_c)(z_i - z_c)] = \sum_{i=1}^4 [(y_i - y_c)(n_c^i - n_c)]$$

$$\frac{\partial n}{\partial x} \sum_{i=1}^4 [(x_i - x_c)(z_i - z_c)] + \frac{\partial n}{\partial y} \sum_{i=1}^4 [(z_i - z_c)(y_i - y_c)] + \frac{\partial n}{\partial z} \sum_{i=1}^4 (z_i - z_c)^2 = \sum_{i=1}^4 [(z_i - z_c)(n_c^i - n_c)]$$

Here, x_i, y_i, z_i are respectively geometric center of neighbor cells, and x_c, y_c, z_c are respectively geometric center of present cell. Present sub-relaxation method^[10] can be written as $\bar{n}_c|_t = \sigma n_c|_t + (1 - \sigma) \bar{n}_c|_{t-\Delta t}$, here, σ is 0.01.

3. Results and discussion

Table 1 shows computational condition from reference [11]. The nitrogen flow is considered in this work. Schematic of grid in simulation is shown in Fig.1. Fig.2 shows computational region. Symmetry conditions in ABCD、ABFE boundary are used, vacuum condition is assumed in CDEF boundary. Cone radius is 6.35mm, half cone angle is 25°, cone length is 50mm. Three kinds of grid size near the wall such like 7.0×10^{-4} m, 5.5×10^{-4} m, 1.5×10^{-4} m signed by Grid1, Grid2, Grid3 are used respectively. The numbers of unstructured cell are 0.63、1.30 and 3.00 millions, respectively. Simulated molecules are 6.00、13.28 and 46.95 millions, respectively.

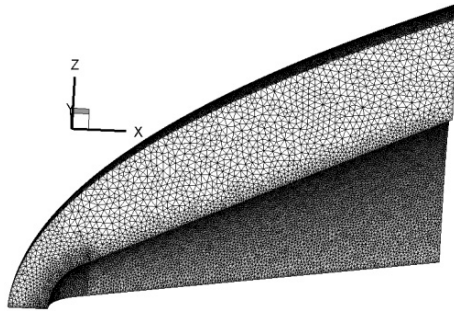


Fig. 1. Schematic of grid in simulation

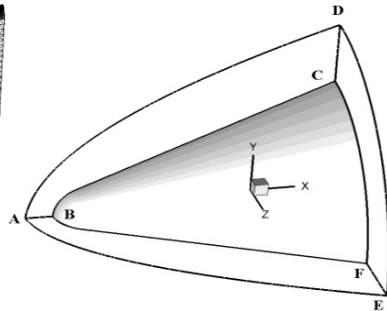


Fig. 2. Domain in simulation

Table1. Experiment condition

Angle of attack	Mach number	Knudsen number	Pressure of free stream	Temperature of free stream	Wall temperature
0	11.3	0.019	21.99Pa	144.44K	297.22K

Fig.3 show pressure contours, temperature contours and velocity contours. It can be found that flow field structures can be captured clearly. Pressure and temperature at stagnation region increase, then decrease along downstream of stagnation owing to expand wave effect. Flow field velocity decreases while passing through shock wave, and a lower velocity region emerges at stagnation region. If grid size is coarser at these great gradient region, collision probability error in cell will bring about and correction need to be done.

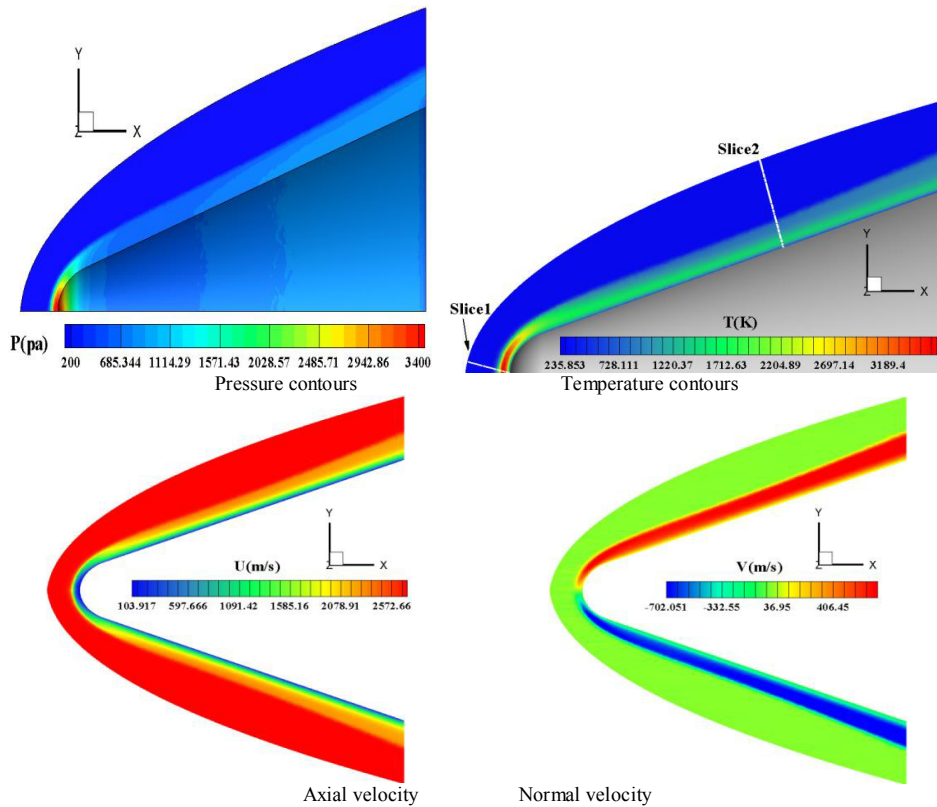


Fig. 3. Flow field contours(Grid size is 5.5×10^{-4})

For validating present code, advanced analysis have been made in Fig.4 and Fig.5 by comparing the results predicted by correction method and no correction method, which show flow temperature contours at slice station in Fig.3. It can be seen that at slice 1 station, the results predicted by correction method at Grid1(a coarse grid size) are consistent with that by no correction at Grid3(a dense grid size), the difference of which is mainly due to number density gradient statistics error and the difficult of capturing flow field gradient at a relative coarse grid size. As can be seen from Fig.4 near the surface, the results predicted by present modified code at Grid1 size also keep an agreement with that predicted by unmodified code at Grid3. The density results near the wall solved by unmodified technique at refined Grid3 and by modified technique at coarse Grid1 is lower than that solved by unmodified code at coarse Grid1. That reduces a lower collision frequency between surface and molecules. It provides a good understanding of the results in Fig. 7, which heat flux decreases near the experimental results as refining grid, and the results predicted by modified code at Grid1, Grid2 are in excellent agreement with experimental results.

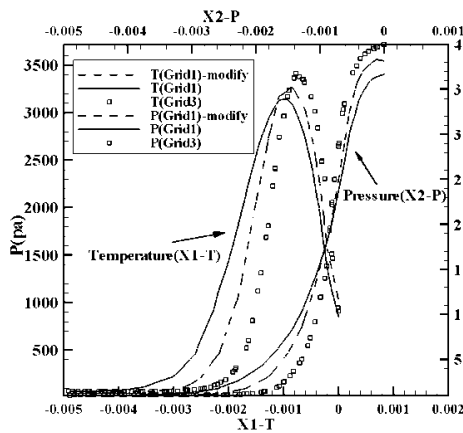


Fig. 4. Flow field distribution line at the slice1

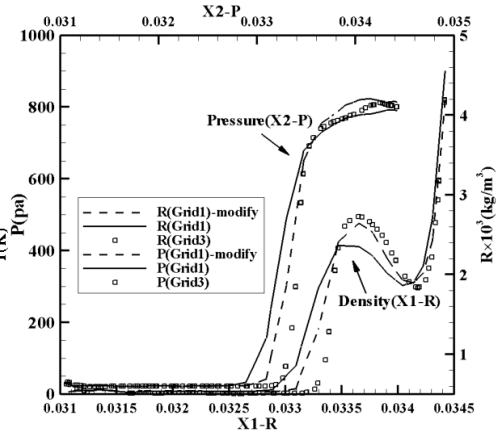


Fig. 5. Flow field distribution line at the slice2

Figure. 6,7 quantify the differences in the surface properties by comparing present method and experiment predictions [11] for pressure and heat flux coefficient, respectively. As can be seen from that, pressure on the surface sharply decreases from stagnation region to its downstream at cone surface, then increases a little under compression effect. Surface pressure decreases on the wake with vacuum outlet boundary, that is similar with flow field structure. The present results predicted by Grid2, Grid3 without any correction of collision probability are consistent with reference [11]'s by comparing the wall pressure coefficient. The results predicted by Grid1 show so much difference from experimental results, but that keeps a good agreement with reference's results while using present correction methods. Heat flux coefficient in fig. 7 shows similar results with pressure coefficient. That is, the agreement between present results without any correction and experimental results become better as refining grid. The results at Grid3 are consistent with experimental results, and surface properties predicted by Grid1, Grid2 without any correction tend to be higher than those by Grid3. Using present correction method, that results predicted by Grid1, Grid2 keep an excellent agreement with computational and experimental results in reference [11]. It can be concluded from fig. 6, 7 that heat flux coefficient variation is more sensitive to grid size than pressure coefficient.

From above all, the present results are consistent with reference's, and present method is credible in DSMC simulation. New correction method can enlarge the local free path limit of grid size, and evidently decreased simulated molecules in all the whole flow field, saved memory, and then improved calculating efficiency in DSMC simulation.

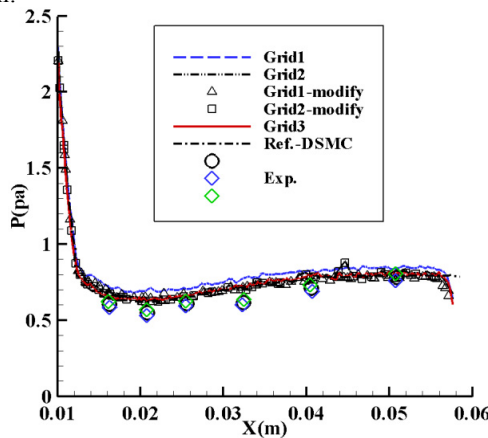


Fig. 6. Pressure distribution along the surface

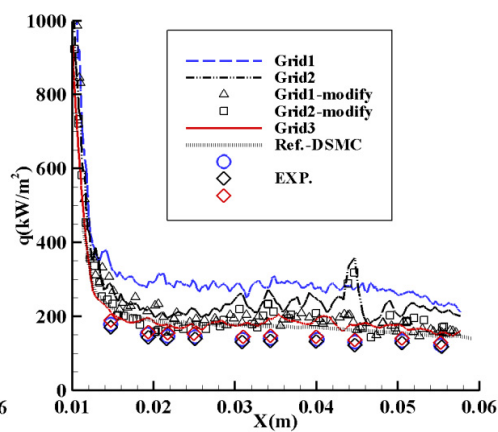


Fig. 7. Heat flux distribution along the surface

4. Conclusions

For correcting collision probability in DSMC simulation at coarse grid size, a new particle collision probability algorithm has been developed to improving DSMC simulation accuracy at coarse grid size. A new modification technique of collision probability with least square method and sub-relaxation technique is introduced based on unstructured tetrahedral cells. A verification case of hypersonic transitional flow around blunt cone validates the modification method. As an ongoing study, it can be extended to three-dimensional transitional flow problems around a complex configuration, which will make the modification a potential use in modern supersonic/hypersonic flight vehicle designs.

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